

PATENT COOPERATION TREATY

From the
INTERNATIONAL SEARCHING AUTHORITY

PCT

To:

see form PCT/ISA/220

WRITTEN OPINION OF THE INTERNATIONAL SEARCHING AUTHORITY (PCT Rule 43bis.1)

Date of mailing
(day/month/year) see form PCT/ISA/210 (second sheet)

Applicant's or agent's file reference
see form PCT/ISA/220

FOR FURTHER ACTION
See paragraph 2 below

International application No.
PCT/US2004/020992

International filing date (day/month/year)
01.07.2004

Priority date (day/month/year)
03.07.2003

International Patent Classification (IPC) or both national classification and IPC
G06F19/00

Applicant
BIOGEN IDEC INC.

1. This opinion contains indications relating to the following items:

- ☒ Box No. I Basis of the opinion
- ☐ Box No. II Priority
- ☒ Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability
- ☐ Box No. IV Lack of unity of invention
- ☒ Box No. V Reasoned statement under Rule 43bis.1(a)(i) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement
- ☐ Box No. VI Certain documents cited
- ☐ Box No. VII Certain defects in the international application
- ☐ Box No. VIII Certain observations on the international application

2. FURTHER ACTION

If a demand for international preliminary examination is made, this opinion will usually be considered to be a written opinion of the International Preliminary Examining Authority ("IPEA"). However, this does not apply where the applicant chooses an Authority other than this one to be the IPEA and the chosen IPEA has notified the International Bureau under Rule 66.1bis(b) that written opinions of this International Searching Authority will not be so considered.

If this opinion is, as provided above, considered to be a written opinion of the IPEA, the applicant is invited to submit to the IPEA a written reply together, where appropriate, with amendments, before the expiration of three months from the date of mailing of Form PCT/ISA/220 or before the expiration of 22 months from the priority date, whichever expires later.

For further options, see Form PCT/ISA/220.

3. For further details, see notes to Form PCT/ISA/220.

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**WRITTEN OPINION OF THE
INTERNATIONAL SEARCHING AUTHORITY**

International application No.
PCT/US2004/020992

Box No. I Basis of the opinion

1. With regard to the **language**, this opinion has been established on the basis of the international application in the language in which it was filed, unless otherwise indicated under this item.
☐ This opinion has been established on the basis of a translation from the original language into the following language , which is the language of a translation furnished for the purposes of international search (under Rules 12.3 and 23.1(b)).
2. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application and necessary to the claimed invention, this opinion has been established on the basis of:
 - a. type of material:
☐ a sequence listing
☐ table(s) related to the sequence listing
 - b. format of material:
☐ in written format
☐ in computer readable form
 - c. time of filing/furnishing:
☐ contained in the international application as filed.
☐ filed together with the international application in computer readable form.
☐ furnished subsequently to this Authority for the purposes of search.
3. ☐ In addition, in the case that more than one version or copy of a sequence listing and/or table relating thereto has been filed or furnished, the required statements that the information in the subsequent or additional copies is identical to that in the application as filed or does not go beyond the application as filed, as appropriate, were furnished.
4. Additional comments:

**WRITTEN OPINION OF THE
INTERNATIONAL SEARCHING AUTHORITY**

International application No.
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Box No. III Non-establishment of opinion with regard to novelty, inventive step and industrial applicability

The questions whether the claimed invention appears to be novel, to involve an inventive step (to be non obvious), or to be industrially applicable have not been examined in respect of:

- ☐ the entire international application,
- ☒ claims Nos. 1-31,37-72

because:

- ☒ the said international application, or the said claims Nos. 1-31,37-72 relate to the following subject matter which does not require an international preliminary examination (*specify*):

see separate sheet

- ☐ the description, claims or drawings (*indicate particular elements below*) or said claims Nos. are so unclear that no meaningful opinion could be formed (*specify*):
- ☐ the claims, or said claims Nos. are so inadequately supported by the description that no meaningful opinion could be formed.
- ☐ no international search report has been established for the whole application or for said claims Nos.
- ☐ the nucleotide and/or amino acid sequence listing does not comply with the standard provided for in Annex C of the Administrative Instructions in that:
 - the written form ☐ has not been furnished
 - ☐ does not comply with the standard
 - the computer readable form ☐ has not been furnished
 - ☐ does not comply with the standard
- ☐ the tables related to the nucleotide and/or amino acid sequence listing, if in computer readable form only, do not comply with the technical requirements provided for in Annex C-bis of the Administrative Instructions.
- ☐ See separate sheet for further details

**WRITTEN OPINION OF THE
INTERNATIONAL SEARCHING AUTHORITY**

International application No.
PCT/US2004/020992

Box No. V Reasoned statement under Rule 43b/s.1(a)(I) with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

1. Statement

Novelty (N)	Yes: Claims	33-36,73-76
	No: Claims	32
Inventive step (IS)	Yes: Claims	
	No: Claims	32-36,73-76
Industrial applicability (IA)	Yes: Claims	32-36,73-76
	No: Claims	

2. Citations and explanations

see separate sheet

Re Item III

Non-establishment of opinion with regard to novelty, inventive step and industrial applicability

1.1 Besides the fact that the following functional statements in independent claim 1:

- **"selecting** a plurality of selected positions ...";
- **"selecting** a plurality of interaction types ...";
- **"... calculating** a value that is indicative of a characteristic ...";
- **"indicating** a characteristic ...";
- **"joining** the information units ...";
- **"joining** the information blocks ...";

and the following in independent claim 37:

- **"conducting** sequence and structural alignments ...";
- **"... to derive** a uniform residue or base numbering system";
- **"identifying** a plurality of selected positions ... **using** one of the uniform residue or base numbering system";
- **"generating** a SIFt ...";
- **"comparing** different SIFt patterns",

do not allow the skilled person to carry out the invention, as no technical details for accomplishing the functions are given, no **technical** effect at all, in the sense of a solution to a technical problem, is derivable from the present form of claims 1-31 and 37-41. Indeed, the subject matter of said claims does not go beyond a mental or administrative procedure as such. Even though the claims refer to target molecules, ligands, proteins, nucleic acids, various interaction types, etc., such references are only to the meaning of the information content in the information blocks of the structural interaction fingerprint and **not** to the solution of a technical problem.

1.2 Claims 42-55 attempt to define a computer-readable data storage medium solely by the information content stored in its database. Said claims therefore relate to presentations of information as such.

- 1.3 Claims 56-72 refer to a computer program for carrying out the method of claims 1-17. However, there is no technical effect derivable from said method and, hence, no technical effect will be generated by the computer program. Claims 56-72, therefore, refer exclusively to a computer program as such.
- 1.4 In other words, claims 1-31 and 37-72 relate to subject matter considered by this Authority to be covered by the provisions of Rule 67.1(iii) PCT (mental acts), Rule 67.1(v) PCT (presentations of information) and Rule 67.1(vi) PCT (computer programs). Consequently, no opinion will be formulated with respect to novelty, inventive step or industrial applicability of the subject matter of said claims (Article 34(4)(a)(i) PCT).

Re Item V

Reasoned statement with regard to novelty, inventive step or industrial applicability; citations and explanations supporting such statement

- 2.1 Reference is made to the following documents:

D1: Briem, H. *et al.* Molecular similarity based on DOCK-generated fingerprints. *J. Med. Chem.* **39**:3401-3408, 1996 (XP002078005);
D2: US-A-2002/072887.

- 2.2 Besides the fact that the following functional statements in independent claim 32:

- "**identifying** a plurality of selected positions ...";
- "**generating** a first structural interaction fingerprint";
- "**generating** a second SIFt ...";
- "**comparing** the first SIFt with the second SIFt to **determine** ...",

do not allow the skilled person to carry out the invention, as no technical details for accomplishing the functions are given, the subject matter of independent claim 32 appears not novel in the sense of Article 33(2) PCT, and therefore the requirements of Article 33(1) PCT are not met.

Indeed, the document D1 discloses (the references in parentheses applying to this document):

A method of predicting the interaction pattern between a target molecule and a test ligand (see abstract), the method comprising:

- identifying a plurality of selected positions between the target molecule and a first ligand, wherein the first ligand is known to bind to the target molecule (see p. 3401 right-hand col. §2; p. 3402 left-hand col. §1; p. 3402 right-hand col. §3);
- generating a first structural interaction fingerprint (see p. 3402 right-hand col. §4);
- generating a second structural interaction fingerprint between the target molecule and a second ligand, the test ligand, by repeating the identifying step and the first structural interaction fingerprint-generating step using the second ligand (see p. 3402 right-hand col. §5-p. 3403 left-hand col. §2: the DOCK score is a structural fingerprint and since this score is compared for molecules A and B it means that also a second structural fingerprint is generated using the same target molecule *h*); and
- comparing the first structural interaction fingerprint with the second structural interaction fingerprint to determine a level of overlapping, wherein a level of overlapping predicts that each of the first and second ligands interacts with the target molecule in a similar pattern (see p. 3403 left-hand col. §2).

Therefore, the subject matter of independent claim 32 is not novel (Article 33(2) PCT).

2.3 Besides the fact that the following functional statements in independent claim 33:

- **"identifying a plurality of selected positions ..."**;
- **"generating a first SIFt of the database"**;

and the following in dependent claims 34 and 35:

- **"analysing** the SIFts ... to **generate** one or more interaction patterns ...";
- **"comparing** one interaction pattern of the database with a SIFt **generated by using** ... thereby **predicting** ...",

do not allow the skilled person to carry out the invention, as no technical details for accomplishing the functions are given, the subject matter of claims 33-36 and 73-76 appears not to involve an inventive step in the sense of Article 33(3) PCT, and therefore the requirements of Article 33(1) PCT are not met.

The subject matter of claims 33-36 relates, as far as understood, to the generation of a database containing structural interaction fingerprints, which is used to generate interaction patterns between the target molecule and the ligands, the database being stored in a computer readable medium. As databases are commonly used for the same purpose in the art of structural fingerprinting (see for instance D2 §§0011-0013), the subject matter of claims 33-36 lacks an inventive step (Article 33(3) PCT).

- 2.4 As the subject matter of claims 73-76 appears to correspond to that of claims 32-36, the subject matter of claims 73-76 also lacks an inventive step (Article 33(3) PCT).